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The Eikonal Equation for Metamaterials Optics from a Moving Boundary Variational Principle

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Abstract—The eikonal equation for inhomogeneous anisotropic metamaterials with equal relative permittivity and permeability tensors ($\bar{\bar{\varepsilon}}(\bar{r}) = \bar{\bar{\mu}}(\bar{r})$) is derived from a free boundary variational principle. An original approach is proposed considering the wavefront as a moving discontinuity surface in an extended continuous media described by the Lagrangian density of electromagnetic fields. The eikonal equation arises as natural (non prescribed) boundary conditions for variational problems.

1. INTRODUCTION

The eikonal equation [1, 2] has been commonly regarded as an asymptotic ($\lambda \to 0$) approximation of wave solutions of Maxwell equations, which is, of course, true. However, in 1964, Luneburg [3] noticed the identity of eikonal equation and the equation of characteristics of Maxwell equations governing propagation of discontinuities of electromagnetic fields. Thus, in Luneburg's approach, propagation of light constitutes a particular class of exact solutions of Maxwell equations, the light rays being curves along which field discontinuities propagate.

In this paper, we follow the Lagrange's old valuable idea of building physical theories from variational principles [4, 5], which have played a relevant role in every field of physics.

Among their advantages, we must mention that *i)* Traditionally in geometrical optics, Fermat's principle is the mathematical tool to find ray trajectories in any material media; *ii)* The functional to be minimized contains all the information about the physics of the system needed to obtain evolution equations and boundary conditions associated with the problem under study; *iii)* Among the most relevant numerical methods in engineering are *direct methods* in the Calculus of Variations; *iv)* Variational principles do not depend on the coordinate system used and this fact gives them their universal character, and finally *v)* The growing importance of control theory and, in particular, optimal control theory, makes the interest in variational calculus grow in many scientific disciplines.

Our aim is to derive the eikonal equation for wavefronts propagation in inhomogeneous anisotropic metamaterials [6–10], assuming that a wavefront can be regarded as a moving discontinuity surface propagating through a continuous medium, similar to a shock wave.

In this paper, the evolution equation of the wavefront, considered as a moving natural boundary of a variational problem, is obtained. It must be emphasized that although evolution equation (ray equation) has been traditionally obtained from Fermat's principle, to our knowledge, derivation of the eikonal equation from natural boundary conditions for the same principle has not been reported.

The paper is structured as follows. In Section 2, the mathematical model of the problem is described. In Subsections 2.1, 2.2, and 2.3, the concepts needed for defining a dual-complementary variational principle are also outlined. Subsection 2.4. is dedicated to systematization of the model. Particularizing for constitutive relations of inhomogeneous metamaterials media (Section 3), a first

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group of wavefront evolution equations is obtained. A dual complementary principle obtained from the co-Lagrangian of the initial problem provides a second group of wavefront evolution equations. Finally, in Section 4, the eikonal equation is derived from these two groups of equations.

2. MATHEMATICAL MODEL

2.1. Generalized Euler-Lagrange Equations

Consider a real linear vector space of functions $\Omega(\phi)$, where inner product $< \phi_1, \phi_2 >$ on $\Omega(\phi)$ is defined to obtain a real Hilbert space: $H(\phi) = \{\Omega(\phi), <,>\}$. Suppose that $I(\phi)$ is a functional $I : \Omega \to R$, defined as:

$$I(\phi_j) = \int_{t_0}^{t} \int_{\tau} \mathscr{L}(\phi_j, T_i\,\phi_j, \overline{r}, t)\, d\tau\, dt \tag{1}$$

where T_i is a linear operator, whose adjoint T_i^* is obtained from the standard definition of inner product ($< \phi_1, \phi_2 >= \int_\tau \int_{t_1}^{t_2} \phi_1\, \phi_2\, d\tau dt$) in Hilbert spaces and generalized Green's theorem [5, 11]:

$$< \phi_1, T\phi_2 >_\Omega = < T^*\phi_1, \phi_2 >_\Omega + \Gamma(\phi_1, \phi_2)_{\partial\Omega} \tag{2}$$

where $\Gamma(\phi_1, \phi_2)_{\partial\Omega}$ denotes boundary terms. As is usual, $\mathscr{L}$ denotes Lagrangian density.

For linear operators used in this paper, application of generalized Green's theorem leads to the following correspondence between adjoint operators:

$$T_1 \equiv \frac{\partial}{\partial t} \Longrightarrow T_1^* = -\frac{\partial}{\partial t}\,;\; T_2 \equiv \text{grad} \Longrightarrow T_2^* = \text{divergence}\,;\; T_3 \equiv \text{curl} \Longrightarrow T_3^* = \text{curl} \tag{3}$$

Following [11], stationary condition $\delta I = 0$ with homogeneous boundary values leads to generalized Euler-Lagrange equations:

$$\frac{\partial \mathscr{L}}{\partial \phi} + \sum_i T_i^* \left(\frac{\partial \mathscr{L}}{\partial\, (T_i\, \phi)} \right) = 0 \quad \text{in } \tau \tag{4}$$

2.2. Hamiltonian and Hamiltonian Equations

Introducing the conjugate variable σ, defined as:

$$\sigma = \frac{\partial \mathscr{L}}{\partial\, (T\, \phi)} \tag{5}$$

where T is any of the linear operators T_i, and Hamiltonian is obtained by means of a Legendre transform:

$$H(\sigma, \phi) = < \sigma, T\phi > - I(\phi) \implies \tag{6}$$

$$I(\sigma, \phi) = \int_{t_0}^{t} \int_{\tau} \left(\sigma(T\phi) - \mathscr{H}(\sigma, \phi) \right)\, d\tau\, dt = \int_{t_0}^{t} \int_{\tau} \left((T^*\sigma)\phi - \mathscr{H}(\sigma, \phi) \right)\, d\tau\, dt \tag{7}$$

where $\mathscr{H}$ denotes Hamiltonian density. Taking into account that I depends on σ and ϕ, stationary condition $\delta I(\sigma, \phi) = 0$ gives:

$$\left\langle T\,\phi - \frac{\partial \mathscr{H}}{\partial\, \sigma} - T^* \left(\frac{\partial \mathscr{H}}{\partial\, (T\, \sigma)} \right),\, \delta\, \sigma \right\rangle + \left\langle T^*\,\sigma - \frac{\partial \mathscr{H}}{\partial\, \phi} - T^* \left(\frac{\partial \mathscr{H}}{\partial\, (T\, \phi)} \right),\, \delta\, \phi \right\rangle = 0 \tag{8}$$

and, consequently, generalized Hamilton equations are obtained:

$$T\,\phi = \frac{\partial \mathscr{H}}{\partial\, \sigma} + T^* \left(\frac{\partial \mathscr{H}}{\partial\, (T\, \sigma)} \right) \tag{9}$$

$$T^*\sigma = \frac{\partial \mathscr{H}}{\partial\, \sigma} + T^* \left(\frac{\partial \mathscr{H}}{\partial\, (T\, \phi)} \right) \tag{10}$$

2.3. Dual Complementary Variational Principle

A new Legendre Transform from the Hamiltonian H leads to the co-Lagrangian F as:

$$F(\sigma, T\,\sigma) =< T^{*}\sigma, \phi > -H(\sigma, \phi) =< T^{*}\sigma, \phi > - < \sigma, T\phi > +I(\phi) \tag{11}$$

which provides a dual-complementary variational principle ($\delta G(\sigma) = 0$) with a new functional $G(\sigma)$ given by:

$$G(\sigma) = \int_{t_0}^{t} \int_{\tau} \mathscr{F}(\sigma, T\,\sigma, \overline{r}, t)\, d\,\tau\, dt \tag{12}$$

2.4. Systematization

Following the works of Tonti [12, 13] on the mathematical structure of physical theories, equation of classical electromagnetism can be decomposed into three sets of equations: definition, balance/evolution and constitutive equations. Thus, one has:

Definition Equations: A group of two homogeneous Maxwell equations:

$$\nabla \times \overline{E} + \frac{\partial\,\overline{B}}{\partial\,t} = 0; \quad \nabla \cdot \overline{B} = 0 \tag{13}$$

which enable us to express fields $\overline{E}$ and $\overline{B}$ in terms of scalar and vector potentials, $\mathscr{V}$ and $\overline{A}$, respectively.

$$\overline{E} = -\nabla\,\mathscr{V} - \frac{\partial\,\overline{A}}{\partial\,t}; \quad \overline{B} = \nabla \times \overline{A} \tag{14}$$

Balance/Evolution Equations: A second group of the remaining Maxwell equations.

$$\nabla \cdot \overline{D} = \rho\,; \qquad \nabla \times \overline{H} = \overline{\jmath} + \frac{\partial\,\overline{D}}{\partial\,t} \tag{15}$$

where ρ and $\overline{\jmath}$ denote the free charge and current, respectively.

Constitutive Equations:

$$\overline{D} = \overline{D}(\overline{E}, \overline{B}); \quad \overline{H} = \overline{H}(\overline{E}, \overline{B}) \tag{16}$$

which, in the case of impedance-matched metamaterials, constitutive equations [6] read:

$$\overline{D} = \varepsilon_0\,\bar{\bar{\varepsilon}}(\overline{r})\,\overline{E}; \quad \overline{B} = \mu_0\,\bar{\bar{\varepsilon}}(\overline{r})\,\overline{H} \tag{17}$$

showing a linear relationship, where relative permittivity/permeability $\bar{\bar{\varepsilon}}$ is a second order symmetric tensor. Since no hypotheses about crystal structure have been made, macroscopic electromagnetic properties of the material model are wholly included in its constitutive equations.

Since there exist duality relations between the groups of Equations (13) and (15), their roles can be interchanged. In this particular case, we assume that these metamaterials are source-free media ($\varrho = 0$ and $\overline{\jmath} = 0$) and therefore the corresponding expresions of scalar and vector potentials are analogous.

3. ANISOTROPIC INHOMOGENEOUS METAMATERIALS

The following approaches, based on energetic arguments and theorems (extremum principles), assign every point of the medium an electromagnetic energy density (free energy) which requires that: the process must be very fast (adiabatic) and differential forms $\overline{D} \cdot \delta\overline{E}$, $\overline{B} \cdot \delta\overline{H}$ and/or their complementary ones:$\overline{E} \cdot \delta\overline{D}$, $\overline{H} \cdot \delta\overline{B}$ be exact. Linear and symmetric constitutive equations (as in the present case) ensure its existence and the expression of Lagrangian density $\mathscr{L}$ for electromagnetic fields can be written as [14]:

$$\mathscr{L} = \frac{1}{2}\left(\overline{E} \cdot \overline{D} - \overline{H} \cdot \overline{B}\right) \tag{18}$$

Taking Equation (13) as definition equations, Equation (17) as constitutive, and according to Equation (18), Lagrangian density can be written in terms of potentials $\mathscr{V}$ and $\overline{A}$ as:

$$\mathscr{L} = \frac{1}{2}\left(\varepsilon_0\,\overline{E} \cdot \bar{\bar{\varepsilon}} \cdot \overline{E} - \frac{1}{\mu_0}\,\overline{B} \cdot \bar{\bar{\varepsilon}}^{-1} \cdot \overline{B}\right) \text{ with } \overline{E} = -\nabla\mathscr{V} - \frac{\partial\overline{A}}{\partial\,t}\ ;\ \overline{B} = \nabla \times \overline{A} \tag{19}$$

Substituting Lagrangian density (Equation (19)) into expression (1), one has:

$$I(\mathscr{V},\overline{A}) = \int_\tau \int_{t_0}^{t} \mathscr{L}\left(\nabla\mathscr{V}, \frac{\partial \overline{A}}{\partial t}, \nabla\times\overline{A}, \overline{r}, t\right) d\tau\ dt \tag{20}$$

where τ defines the spatial domain.

First, it is easy to verify that the remaining Maxwell equations (given in Equation (15)) arise directly as generalized Euler-Lagrange equations for electromagnetic fields with Lagrangian density (19) assuming prescribed boundary and initial conditions.

However, in this work, a radically different approach is proposed: We consider that the spatial definition domain τ of electromagnetic field functional (20) has a moving boundary $\partial\tau \equiv S(\overline{r},t) = 0$ (S being the eikonal) which behaves as a closed material surface surrounding the region disturbed by electromagnetic fields. Moreover, for our purposes, an analytical extension of the problem is performed. Thus, the definition domain is extended to the whole space (E^3) with the requirement of homogeneous boundary conditions at infinity and assuming that the wavefront behaves as a moving surface surrounding, at all times, the variable and finite domain τ. This procedure is performed with the aid of Heaviside (or step) distribution Θ. Then the problem comes down to find the extremal of:

$$I = \int_{t_0}^{t}\int_\tau \mathscr{L}\, d\tau\, dt = \iint_{E^3\times T} \mathscr{L}(\phi, T_i\phi, \overline{r}, t)\,[1-\Theta(S(\overline{r},t))]\, d\tau\, dt \tag{21}$$

where it is assumed that:

$$\Theta(S(\overline{r},t)) = \begin{cases} 0, & \text{for } \overline{r} \text{ inside } \tau \\ 1, & \text{for } \overline{r} \text{ outside } \tau \end{cases} \tag{22}$$

Since Heaviside (Θ) and Dirac delta ($\hat{\delta}$) distributions verify that [15–18]:

$$\hat{\delta}(\phi(x)) = \frac{D\,\Theta(\phi(x))}{D\,\phi}; \quad \nabla\Theta = \hat{\delta}(\phi(x))|\nabla\phi|; \quad \frac{\partial\Theta}{\partial t} = \hat{\delta}(\phi(x))\left|\frac{\partial\phi}{\partial t}\right| \tag{23}$$

Consequently, δI takes the expression:

$$\begin{aligned}\delta\int_{t_0}^{t}\int_\tau \mathscr{L} d\tau dt \; = \; & \iint_{E^3\times T}\left(\frac{\partial\mathscr{L}}{\partial\phi} - \sum_i T_i\left(\frac{\partial\mathscr{L}}{\partial(T_i\phi)}\right)\right)[1-\Theta(S)]\delta\phi d\tau dt \\ & + \iint_{E^3\times T}\sum_i T_i\left(\frac{\partial\mathscr{L}}{\partial(T_i\phi)}[1-\Theta(S)]\delta\phi\right) d\tau dt \\ & - \iint_{E^3\times T}\sum_i \frac{\partial\mathscr{L}}{\partial(T_i\phi)} T_i(S)\hat{\delta}(S)\delta\phi d\tau dt \end{aligned} \tag{24}$$

It is easy to verify that the second term of the sum vanishes by considering homogeneous boundary conditions at infinity, where every field tends to zero. Stationarity condition $\delta I = 0$ provides two kinds of equations: *a)* Generalized Euler Lagrange equations:

$$\frac{\partial\mathscr{L}}{\partial\phi} - \sum_i T_i\left(\frac{\partial\mathscr{L}}{\partial(T_i\phi)}\right) = 0 \tag{25}$$

which hold in domain τ and represent the *ray evolution equations*.

b) Taking into account Dirac-delta $\hat{\delta}$ properties, expression

$$\iint_{E^3\times T}\sum_i \frac{\partial\mathscr{L}}{\partial(T_i\phi)}\, T_i(S)\,\hat{\delta}(S)\,\delta\phi\, d\tau\, dt = 0 \tag{26}$$

leads to the natural boundary condition [19].

$$\sum_i \frac{\partial\mathscr{L}}{\partial(T_i\phi)}\Big|_{S(\overline{r},t)} T_i(S) = 0 \tag{27}$$

which when applied to potentials and operators enables us to obtain *eikonal equation*, as we shall see below. Thus, applying Equation (27) to Lagrangian density Equation (19) for the scalar potential $\mathscr{V}$, one has that:

$$[\overline{D}] \cdot \nabla S = 0 \tag{28}$$

where [] denotes the "jump" or discontinuity in the vector field. In an analogous manner, application of natural boundary conditions (27) to a generic component A_i of vector potential $\overline{A}$ yields:

$$[\overline{D}]\,\frac{\partial S}{\partial t} - \nabla S \times [\overline{H}] = 0 \tag{29}$$

In order to obtain the two remaining wavefront evolution equations, roles of Equations (13) and (15) are interchanged. So we take the former evolution Equation (15) as new definition equations. The procedure developed above enables us to obtain co-Lagrangian density (dual to the Lagrangian density). In fact, as is usual in physics, we seek conjugate variable with respect to linear operator $\partial\overline{A}/\partial t$:

$$\sigma_i = \frac{\partial \mathscr{L}}{\partial \dot{A}_i} = -D_i \tag{30}$$

as well as Hamiltonian density, which has the expression:

$$\mathscr{H} = -\overline{D} \cdot \overline{A} - \mathscr{L} = \frac{1}{2\,\varepsilon_0}\,\overline{D} \cdot \bar{\bar{\varepsilon}}^{-1} \cdot \overline{D} + \frac{1}{2\,\mu_0}\,\overline{B} \cdot \bar{\bar{\varepsilon}}^{-1} \cdot \overline{B} + \nabla \cdot (\mathscr{V}\,\overline{D}) \tag{31}$$

where $\nabla\mathscr{V} \cdot \overline{D} = \nabla \cdot (\mathscr{V}\,\overline{D})$, because $\nabla \cdot \overline{D} = 0$ in charge free media.

So, fields $\overline{D}$ and $\overline{H}$ can be expressed in terms of other electromagnetic potentials, say ψ and $\overline{R}$, as:

$$\overline{H} = \nabla\,\psi + \frac{\partial\,\overline{R}}{\partial\,t}\,; \qquad \overline{D} = \nabla \times \overline{R} \tag{32}$$

and co-Lagrangian density is introduced from Hamiltonian density by means of a Legendre transform:

$$\mathscr{F}\left(\overline{D}, \frac{\partial\,\overline{D}}{\partial\,t}\right) = -\overline{A} \cdot \frac{\partial\,\overline{D}}{\partial\,t} - \mathscr{H}(\overline{D}, \overline{A}) \tag{33}$$

Elementary calculations yield:

$$\mathscr{F}\left(\overline{D}, \frac{\partial\,\overline{D}}{\partial\,t}\right) = \frac{1}{2}\left(\mu_0\,\overline{H} \cdot \bar{\bar{\varepsilon}} \cdot \overline{H} - \frac{1}{\varepsilon_0}\,\overline{D} \cdot \bar{\bar{\varepsilon}}^{-1} \cdot \overline{D}\right) + \nabla \cdot (\overline{A} \times \overline{H}) \tag{34}$$

and then, co-Lagrangian is given by:

$$F = \int_\tau \frac{1}{2}\left(\mu_0\,\overline{H} \cdot \bar{\bar{\varepsilon}} \cdot \overline{H} - \frac{1}{\varepsilon_0}\,\overline{D} \cdot \bar{\bar{\varepsilon}}^{-1} \cdot \overline{D}\right) + \int_{\partial\tau} (\overline{A} \times \overline{H}) \cdot d\overline{\Sigma} \tag{35}$$

where Gauss' theorem has been applied, and $d\overline{\Sigma}$ denotes a surface element at the boundary $\partial\tau$. Then the problem is to obtain extremals of the functional:

$$G = \int_{t_0}^{t} \int_\tau \mathscr{F}\,d\,\tau\,dt \tag{36}$$

with free boundary conditions.

Following a procedure analogous to the previous one, it must be noticed that: *i)* The remaining group of Maxwell equations (in this case, those given by Equation (13)) arise now from the application of the generalized Euler-Lagrange Equation (4) to the new functional G (36) with prescribed boundary and initial conditions; *ii)* Application of the analytical expansion to the whole space:

$$\delta G = \delta \int_{E^3 \times T} \mathscr{F}\,[1 - \Theta(S(\overline{r}, t)]\,d\,\tau\,dt \tag{37}$$

leads to the following wavefront evolution equations from natural boundary conditions (27):

$$[\overline{B}] \cdot \nabla S = 0; \quad [\overline{B}]\,\frac{\partial\,S}{\partial\,t} + \nabla\,S \times [\overline{E}] = 0 \tag{38}$$

4. EIKONAL EQUATION

Using the two non-trivial Equations (29) and (38):

$$[\overline{B}]\,\frac{\partial S}{\partial t} + \nabla S \times [\overline{E}] = 0\ ;\ [\overline{D}]\,\frac{\partial S}{\partial t} - \nabla S \times [\overline{H}] = 0 \tag{39}$$

and eliminating field variables $\overline{E}$, $\overline{D}$, $\overline{B}$ and $\overline{H}$, the eikonal equation follows immediately.

Thus, we must take into account the mathematical property [20] that says: For all vectors $\overline{a}$, $\overline{b}$ and any invertible tensor $\bar{\bar{A}}$:

$$(\bar{\bar{A}} \cdot \overline{a}) \times (\bar{\bar{A}} \cdot \overline{b}) = (\det \bar{\bar{A}})\, \bar{\bar{A}}^{-1} \cdot (\overline{a} \times \overline{b}) \tag{40}$$

and according to constitutive equations of these media (17), one can write:

$$\overline{D} \times \overline{B} = \frac{1}{c^2}(\bar{\bar{\varepsilon}} \cdot \overline{E}) \times (\bar{\bar{\varepsilon}} \cdot \overline{H}) = I_3\, \bar{\bar{\varepsilon}}^{-1} \cdot (\overline{E} \times \overline{H})/c^2 \tag{41}$$

where $I_3 = \varepsilon_1\, \varepsilon_2\, \varepsilon_3$ is the determinant of tensor $\bar{\bar{\varepsilon}}$ (product of its eigenvalues).

From equations given in Equation (39) and using the expression (41), the eikonal equation for these media is immediately derived, as shown in [21]:

$$\nabla S \cdot \bar{\bar{\varepsilon}} \cdot \nabla S = \frac{I_3}{c^2}\left(\frac{\partial S}{\partial t}\right)^2 \tag{42}$$

5. CONCLUSIONS

A novel presentation (to our knowledge) of wavefront evolution equation from variational principles in optics of one specific inhomogeneous anisotropic metamaterial medium is discussed.

(i) Field equations (including constitutive equations) defined for a given instant in a finite geometric domain are extended to the whole space, using distributions, in order to obtain vanishing boundary conditions at infinity.

(ii) The linear character of constitutive equations enables us to define a complementary electromagnetic energy, and consequently, two dual complementary variational principles are stated, which make it possible to obtain two sets of Maxwell equations, in such a way that the definition equations of every principle are the extremals of the other. To summarize, each group of Maxwell equations can be considered the dual of the other group with respect to variational principles.

(iii) The passage from one variational principle to the other is performed according to standard procedures from continuum mechanics by means of two successive Legendre transforms, passing from Lagrangian density to co-Lagrangian.

(iv) Once the problem is reduced to finding the extremal of a functional, powerful numerical calculation tools inherent to variational principles (like direct methods) can be applied. The main advantage of this approach is precisely the extremal character of the functional. This methodology is widely used in other scientific fields like image theory, where it provides a procedure to eliminate the noise with "scientific arguments" avoiding "emotional criteria" [15–18].

(v) The most relevant and original contribution is that it has been demonstrated, by means of variational principles, that the eikonal equation is an exact solution of Maxwell equations arising as a natural boundary condition for these principles.

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